Numerical Treatment of ODE

- remember population dynamics: one or some ODE
  - there as an **initial value problem**: starting point given
  - sometimes also as a **boundary value problem**: starting and final point given (think of a space shuttle's trajectory, e.g.)
- prototypes of an initial value problem (IVP):

$$\dot{y}(t) = f(t, y(t)), \quad y(a) = y_a, \quad t \geq a$$

$$\dot{y}_i(t) = f_i(t, y_1(t), \ldots, y_n(t)), \quad y_i(a) = y_{i,a}, \quad t \geq a, \quad i = 1, \ldots, n$$

- if f depends on t only: simple integration or *quadrature*
- standard approach for IVP: **finite difference** approximation (difference quotient instead of derivative) $y(a+\delta t) \doteq y(a) + \delta t \cdot f(t, y(a))$

$$y_{k+1} = y_k + \delta t \cdot f(t_k, y_k), \quad t_k = a + k\delta t, \quad k = 0,1,\ldots$$

Euler's Method, Discretization Error

- this is the simplest strategy and called *Euler's method*
- other derivation: truncated Taylor expansion of y(t)

$$y(t_{k+1}) = y(t_k) + (t_{k+1} - t_k)\dot{y}(t_k) + R \doteq y(t_k) + (t_{k+1} - t_k) f(t_k, y_k)$$

- **local discretization error**: local influence of using differences instead of derivatives; here:

$$l(\delta t) = \max_{[a,b]}\{(y(t+\delta t) - y(t))/\delta t - f(t, y(t))\}$$

- **global discretization error**: maximum error of all computed discrete approximations:

$$e(\delta t) = \max_{[a,b]}\{|y_k - y(t_k)|\}$$

- **consistency**: $l(\delta t) \to 0 \text{ for } \delta t \to 0$
- **convergence** (stronger): $e(\delta t) \to 0 \text{ for } \delta t \to 0$

Order of Convergence

- Euler (some restrictions with respect to y and f):
  - consistent of *first order*: $l(\delta t) = O(\delta t)$
  - convergent of *first order*: $e(\delta t) = O(\delta t)$
  - There are methods that are consistent but do not converge!
- look for higher-order methods (faster convergence)
  - start from Taylor expansion: leads to complicated formulas (higher derivatives of f) ☹
  - use aditional evaluations of f: Runge-Kutta-type methods
- simplest representative: method of Heun

$$y_{k+1} = y_k + \frac{\delta t}{2}\left(f(t_k, y_k) + f(t_{k+1}, y_k + \delta t \cdot f(t_k, y_k))\right)$$

- both consistent and convergent of second order

Method of Runge and Kutta

- most famous representative: Runge-Kutta method

$$y_{k+1} = y_k + \frac{\delta t}{6}(T_1 + 2T_2 + 2T_3 + T_4),$$

$$T_1 = f(t_k, y_k),$$

$$T_2 = f\left(t_k + \frac{\delta t}{2}, y_k + \frac{\delta t}{2} T_1\right),$$

$$T_3 = f\left(t_k + \frac{\delta t}{2}, y_k + \frac{\delta t}{2} T_2\right),$$

$$T_4 = f\left(t_{k+1}, y_k + \delta t\, T_3\right)$$

- consistent and convergent of fourth order
- Euler/Heun/Runge-Kutta correspond to rectangle/trapezoidal/Simpson quadrature!

Alternative: Multistep Methods

- Runge-Kutta-type methods are expensive ☹: many evaluations of f (sometimes not given in closed form)
- different way to get higher order by profiting from history: Adams-Bashforth-type or multistep methods
  - prominent representative: second-order method

$$y_{k+1} = y_k + \frac{\delta t}{2}\left(3 f(t_k, y_k) - f(t_{k-1}, y_{k-1})\right)$$

  - general form: take polynomial P(t) interpolating f in the discrete points of time

$$y_{k+1} = y_k + \int_{t_k}^{t_{k+1}} \dot{y}(t)\,\mathrm{d}\,t = y_k + \int_{t_k}^{t_{k+1}} f(t, y(t))\,\mathrm{d}\,t \doteq y_k + \int_{t_k}^{t_{k+1}} P(t)\,\mathrm{d}\,t$$

  - p=1: Euler; p=2: above method; generally: order p
  - start: no/not enough predecessors available; hence modify!

Implicit Methods

- All schemes mentioned so far are *explicit* ones: The rule shows a direct way to do another time step.
- now: use the new value y_{k+1} on the right-hand side, too
- This leads us to Adams-Moulton multistep schemes:
  - use interpolation and previous values as with Adams-Bashforth
  - second order variant:

$$y_{k+1} = y_k + \frac{\delta t}{2}\left(f_k + f_{k+1}\right)$$

  - fourth order variant:

$$y_{k+1} = y_k + \frac{\delta t}{24}\left(f_{k-2} - 5 f_{k-1} + 19 f_k + 9 f_{k+1}\right)$$

- How to get y_{k+1} in the implicit case?
  - straightforward way: solve the (generally nonlinear) equation
  - easier (and widespread): *predictor-corrector* approach

Ill-Conditioned Problems

- small changes in input entail completely different results
- Numerical treatment of such problems is difficult!
- an example:
  - consider the ODE $\ddot{y}(t) - N \cdot \dot{y}(t) - (N+1) \cdot y(t) = 0$
  - initial conditions: $y(0) = 1, \quad \dot{y}(0) = -1$
  - exact solution: $y(t) = e^{-t}$
- slight change in initial condition:
  - new value of y in t=0: $y_\varepsilon(0) = 1 + \varepsilon$
  - resulting new solution: $y_\varepsilon(t) = \left(1 + \frac{N+1}{N+2}\varepsilon\right)e^{-t} + \frac{\varepsilon}{N+2}e^{(N+1)t}$
  - arbitrarily small change leads to completely different result: $t \to \infty$
- risk: non-precise input, round-off errors, ...

Stability

- consider another IVP: $\dot{y}(t) = -2y(t) + 1, \quad y(0) = 1$
- exact solution: $y(t) = \left(e^{-2t} + 1\right)/2$
- well-conditioned: $y_\varepsilon(0) = 1 + \varepsilon \quad \Rightarrow \quad y_\varepsilon(t) - y(t) = \varepsilon\, e^{-2t}$
- use the midpoint rule: $y_{k+1} = y_{k-1} + 2\delta t \cdot f_k$

  $$y_{k+1} = y_{k-1} + 2\delta t\left(-2y_k + 1\right) = y_{k-1} - 4\delta t \cdot y_k + 2\delta t, \quad y_0 = 1$$
- 2-step rule: start with initial value and the exact $y(\delta t)$
  - time step $\delta t = 1.0 \Rightarrow y_9 = -4945.5, \quad y_{10} = 20953.9$
  - time step $\delta t = 0.1 \Rightarrow y_{79} = -1725.3, \quad y_{80} = 2105.7$
  - time step $\delta t = 0.01 \Rightarrow y_{999} = -154.6, \quad y_{1000} = 158.7$
- midpoint rule is second-order consistent, but does not converge here: oscillations or instable behaviour
- there are stability conditions; generally:

  consistency + stability = convergence

Stiffness

- for another phenomen, consider the IVP

$$\dot{y}(t) = -1000y(t) + 1000, \quad y(0) = y_0 = 2$$

- exact solution: $y(t) = e^{-1000t} + 1$
- problem well-conditioned
- explicit Euler: stable (as all explicit 1-step methods or all Adams-Bashforth or all s-step Adams-Moulton methods for s>1 are)

$$y_{k+1} = y_k + \delta t(-1000y_k + 1000) = (1 - 1000\delta t)y_k + 1000\delta t$$
$$= (1 - 1000\delta t)^{k+1} + 1$$

- oscillations and divergence for $\delta t > 0.002$
- Why that? Consistency and stability are *asymptotic* terms. Remedy: Implicit methods (try implicit Euler)!

Boundary Value Problems: Outlook

- example: $\ddot{y} = f(t, y, \dot{y}),\ t_a \le t \le t_b,\ y(t_a) = y_a,\ y(t_b) = y_b$
- special case: $\ddot{y}(t) = a(t)\dot{y}(t) + b(t)y(t) + c(t)$, same b.c.
- a vanishing and b positive: BVP has unique solution
- discrete grid: $\delta t = (t_b - t_a)/n,\ t_0 = t_a,\ t_n = t_b,\ t_i = t_a + i\delta t$
- finite difference approximation for second derivative:

$$\ddot{y}(t) \doteq \frac{y(t+\delta t) - 2y(t) + y(t - \delta t)}{\delta t^2}$$

- discrete analogon to ODE in each grid point:

$$\delta t^{-2} \cdot (y_{i+1} - 2y_i + y_{i-1}) - b_i y_i = c_i, \quad i = 1, \ldots, n-1$$

- tridiagonal system of linear equations
- alternative: shooting methods (reduction to IVPs)